Influence Of $\text{SiN}_x$: H And $\text{SiO}_x$ Films On Optical And Electrical Properties Of Antireflective Coatings For Silicon Solar Cells

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ABSTRACT: To increase the photon transmission in solar cells based on multicrystalline silicon, two different double layer antireflections (DARC, and DARC$_2$) were optimized and simulated, to optimize the antireflection double layer, we have developed a numerical simulation code with Matlab software package where we have used the method of transfer matrix to solve the optical equation. These solutions permit us to plot the optical reflectivity and the absorption versus wavelengths and layer thicknesses. The optical refractive index and thicknesses of considered materials which allowed us to have the best results of reflection were used to simulate the electrical properties of the cell with PC1D software. Thus, our results showed that the average reflectivity of 5.4 % and 6.4 % is obtained with a DARC$_1$, composed of two different layers of hydrogenated silicon nitride (SiN$_x$: H) and silicon oxide (SiO$_x$) and DARC$_2$, composed of two layers of silicon nitride hydrogenated SiN$_2$: H with optical indexes and thicknesses different, respectively. These optimized structures have the potential to increase the short-circuit current by more than 1.8% with a DARC$_1$ and up 3.3 % with a DARC$_2$ for non-encapsulated cells, in comparison with the standard single SiN$_2$: H ARC.

Keywords: AR coating, Silicon-Nitride, Silicon-Oxy-nitride, solar cells

1. Introduction
Optical losses strongly affect the power delivered by the photovoltaic cell decrease in the short circuit. For this, the use of an antireflection coating (CAR), combined with the texturing of the silicon substrate, significantly reduces the losses. For ten years, depositing an antireflection coating of silicon nitride hydrogenated SiN$_x$: H (SiN$_x$) has emerged as CAR least because its refractive index can be easily adjusted. It is an effective and inexpensive way to ensure low reflectivity and a better passivation of silicon solar cells. However, for a simple zero reflectivity antireflection layers (SCAR) can take place only for a single wavelength, since the layer acts as a quarter wave plate and it depends on the wavelength. For this application of a double layer Antireflection (DARC) combining two materials SiN/SiN$_x$, SiO$_2$/Si$_3$N$_4$, and ZnS/MgF$_2$ [1, 2, 3] on the front is a very promising avenue. The refractive index n and extinction coefficient k of SiN increase with the level of silicon in the layer [4]. Thus, it can vary from 1.9 to 3.0. The optimal optical index of a transparent antireflection layer of non-encapsulated solar cell silicon is 2.05 and about 2.4 for an encapsulated solar cell (glass, acetate and EVA). According to Soppe and al [5], the best efficiency of solar cells is obtained for optical low refractive indexes. However, surface passivation becomes better for indexes above 2.3 and the bulk passivation is good for a refractive index between n = 2.1 and 2.2. To combine between the minimization of the reflectivity and a good passivation on the surface, one first approach consists to use a double antireflection layer with two materials of different refractive index n: a lower layer relatively rich in silicon to allow good surface passivation and a top layer of low refractive index to minimize reflection at the surface of the solar cell [6].

This work is to find the best configurations of double antireflection coatings (DARC) can effectively improve the electrical performance and spectral solar cells. For this we chose two different DARC. The DARC$_1$ and the DARC$_2$ form of two different materials SiN/ SiN$_x$ and SiN$_x$/SiO$_x$, respectively. In this work, the absorption of DARC (A ≠ 0) and the thickness $d_2$ of the SiN$_x$: H layer is higher than 30 nm which is the minimal limit required ensuring a good passivation surface according to Lauinger et al. [7]. The theory of antireflection coating is examined by many authors [6, 8, 9]. The transfer matrix method [11] is usually employed for calculation of reflection coefficient. In this paper, we present the result of calculation obtained by our computer program of SARC, DARC$_1$ and DARC$_2$ on silicon substrate.

2. Optical modeling
In this work we have used Matlab software to simulate ARC structures and calculate their reflectance spectra. The ARC structures were simulated for the wavelength 610 nm. Reflection spectra were simulated for wavelengths from 300 to 1100 nm and at an incidence angle of 90°. The transfer matrix method (TMM) [11] is usually employed for calculation of reflection coefficient.

3. Modeling
The multilayer system shown in the Fig.1 is annotated by the electric field components at each interface. The Index indicates the layers. The signs ‘+’ and ‘-’ can distinguish the incident and reflected waves, respectively. The Signs are used to distinguish the waves are at the right interface to those on his left.

![Fig.1. Multilayer structure used to illustrate the principle of TMM.](image-url)
The multilayer structure consists of \( N + 1 \) interfaces and \( N \) layers, besides the layer to the extreme left represented generally by air \( (n_0 = 1) \) and the far right which forms the substrate (base silicon). The layers are characterized by refractive indexes \( n_i \) as shown in Fig.1. The boundary conditions for the vectors of the electric field \( E \) in each side of any interface allows a simple description by a \( 2 \times 2 \) matrix. Thus, for the \( m \)th interface, the relationship between the components of the field is given by (1) [10]:

\[
\begin{pmatrix}
E_{m+1}^+ \\
E_{m+1}^-
\end{pmatrix} = Q_{m-1} Q_m
\begin{pmatrix}
E_m^+ \\
E_m^-
\end{pmatrix}
\]

(1)

With

\[
Q_{m-1} Q_m = \frac{1}{r_{m-1,m}} \begin{pmatrix}
1 & r_{m-1,m} \\
r_{m-1,m} & 1
\end{pmatrix}
\]

(2)

The product \( Q_{m-1} Q_m \) of the dynamical matrices (the so-called refraction or transmission matrix, \( Q_{m-1,m} \) of the interface) is a \( 2 \times 2 \) matrix, and when expressed in terms of the complex Fresnel reflection, \( r_{m-1,m} \), and transmission, \( t_{m-1,m} \), coefficients of the interface, it takes the same form in both cases of \( s \) or \( p \) waves [10].

\[
r_{m-1,m} = \frac{n_{m-1} - n_m}{n_{m-1} + n_m} \quad \text{and} \quad t_{m-1,m} = \frac{2 n_{m-1}}{n_{m-1} + n_m}
\]

(3)

The field components at the left and right of the \( m \)th layer are bonded by the propagation matrix \( P_m \)

\[
\begin{pmatrix}
E_{m+1}^+ \\
E_{m+1}^-
\end{pmatrix} = P_m \begin{pmatrix}
E_m^+ \\
E_m^-
\end{pmatrix}
\]

(4)

With

\[
P_m = \begin{pmatrix}
\exp(i \delta_m) & 0 \\
0 & \exp(-i \delta_m)
\end{pmatrix}
\]

(5)

Where \( \delta_m = \frac{2 \pi}{\lambda} n_m d_m \) is the phase difference, \( n_m \) is the index of the layer and \( d_m \) is the thickness of the layer, \( \lambda \) is the wavelength in nm and \( j^2 = -1 \). An iterative application of the transformations above for the \( N \) layers and \( N+1 \) interface will lead to a multiplication of \( (N+1) \) matrices \( (2 \times 2) \).

\[
\begin{pmatrix}
E_0^+ \\
E_0^-
\end{pmatrix} = H \begin{pmatrix}
E_{N+1}^+ \\
E_{N+1}^-
\end{pmatrix}
\]

(6)

With \( H \) is the transfer matrix of the system

\[
H = \begin{bmatrix}
H_{11} & H_{12} \\
H_{21} & H_{22}
\end{bmatrix} = Q_N Q_{N-1} \cdots Q_2 Q_1
\]

(7)

\( H_{ij} \) are the elements of the characteristic matrix of the multilayer. Include components of the incident field, reflected and transmitted respectively

\[
E_i = E_0^+, \quad E_r = E_0^- \quad \text{et} \quad E_t = E_{N+1}^-
\]

(8)

Note that these quantities are generally complex. The coefficients of reflection and transmission are determined below. Assuming that

\[
E_0^+ = E_{N+1}^- = 0
\]

In terms of components of the transfer matrix, \( r \) and \( t \) can be written by the following relationships

\[
r = \frac{E_x}{E_x} = \frac{E_{21}}{E_{11}} \quad \text{and} \quad t = \frac{E_{22} + j E_{21}}{E_{11}}
\]

(9)

The conservation of energy gives:

\[
|S_o|^2 = |S_o|^2 + |S_{N+1}^-|^2 + A = \frac{|E_x|^2}{2 n_0} = \frac{|E_x|^2}{2 n_0} + \frac{|E_{N+1}^+|^2}{2 n_{N+1}} + A
\]

(10)

With \( A \) absorption layer and \( n_0 = \sqrt{\varepsilon_0} \)

\( \varepsilon_0 \) and \( \mu_0 \) are the permittivity and permeability of the space. It gives me:

\[
|E_x|^2 = \frac{(|r|^2 |E_x|^2 + |t|^2 |E_x|^2)^2}{2 n_0} + A \Rightarrow |r|^2 + |t|^2 \left( \frac{n_0}{n_{N+1}} \right) = 1
\]

(11)

For a medium without losses and nonmagnetic (Devoid magnetic properties), we

\[
|r|^2 + |t|^2 \left( \frac{n_{N+1}}{n_0} \right) + A = 1
\]

(12)

and consequently

\[
R = |r|^2 \quad \text{and} \quad T = |t|^2 \left( \frac{n_{N+1}}{n_0} \right)
\]

(13)

With \( R + T + A = 1 \)

(14)

The absorption coefficient \( \alpha \) is defined by the following equation.

\[
\alpha = \frac{4 \pi k}{\lambda}
\]

(15)

4. Optical results

4.1. Reflection single layer coating

For a single layer antireflection based SiN, the reflectivity of this layer is a function of \( n \) and \( d \). The minimum reflection of 11.7% can be achieved with a layer of \( n = 2.03 \) and \( d = 73 \) nm (fig.2.). This value can be reduced to a solar cell with a textured surface.

Fig 2. Reflection losses as a function of wavelengths of SARC (n=2.03, d=73 nm)
These calculations show that, in most cases, the silicon nitride is not sufficient to cover the range of refractive indices appropriate. For this reason, we decided to study a combination of SiN and silicon oxide SiO$_2$, to obtain refractive index between $n = 1.46$ (SiO$_2$) and $n = 1.9$ (SiN). However, some combination with high refractive indices which allowed us to reduce the reflectivity will inevitably induce a strong absorption.

4.2. Reflection double layer coating

The principle of double layer antireflective is based on the filing of an upper layer with a small refractive index which reduced reflectivity in the UV range and the filing of a lower layer with a large index to reduce the reflectivity in the range of visible and IR. The optimized reflectance was simulated and correlated with the incident and the total losses caused by reflected photon (see Fig. 3, Fig. 4.) for DARC$_1$ (SiN-SiN) with $n_1 = 1.9$, $n_2 = 2.5$, $d_1 = 58$ nm, $d_2 = 43$ nm and DARC$_2$ (SiN-SiO$_2$) $n_1 = 1.5$, $n_2 = 2.2$, $d_1 = 76$ nm and $d_2 = 48$ nm (Table 1).

<table>
<thead>
<tr>
<th></th>
<th>$n_1$</th>
<th>$d_1$(nm)</th>
<th>$n_2$</th>
<th>$d_2$(nm)</th>
<th>$R_{eff}$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SARC</td>
<td>2.0</td>
<td>73</td>
<td>-</td>
<td>-</td>
<td>11.7</td>
</tr>
<tr>
<td>DARC$_1$ (SiN-SiN)</td>
<td>1.9</td>
<td>58</td>
<td>2.5</td>
<td>43</td>
<td>6.4</td>
</tr>
<tr>
<td>DARC$_2$ (SiO$_2$-SiN)</td>
<td>1.5</td>
<td>76</td>
<td>2.2</td>
<td>48</td>
<td>5.4</td>
</tr>
</tbody>
</table>

The minimum of reflectivity corresponds with wavelength at which the $n$ and $d$ of the layers causes a phase shift of $\pi$ on the light which is reflected between the various interfaces of the layers which are 750 nm and 320 nm for DARC$_1$ and 640 nm and 320 nm for DARC$_2$, this phase shift shout of interfere destructively and engenders a complete absorption or transmission of these wavelengths.

For a double layer antireflective (DARC$_1$) based SiN, the reflectivity is reduced to 6.4% fig.3, but the losses are still important for wavelengths $< 600$ nm which is due to the refractive index of the layer SiN and it represents 89% of total losses by reflection photon flux $F(\lambda)$ of the solar spectrum AM 1.5 G. The solution to this problem is the filing of a DARC$_2$ composed of SiO$_2$ with a refractive index $n$ small. These layers are easily filed with the PECVD method. Using a DARC$_2$ reduced the total reflectivity to 5.4% and reduces the reflectivity for wavelengths $< 600$ nm relative to the DARC$_1$ which represents a loss of 57% of total flux lost fig. 4.

4.3. Absorption

The absorption in the antireflective layers coating strongly affects the solar cells. The fig.5 watch the absorption of the DARC$_1$ and DARC$_2$ according to the wavelength, these losses are particularly in the range of UV, that is caused by the optical index of the layers superior (SiN) as of these double layers. The DARC$_1$ is more absorbing (1.2%) that the DARC$_2$ (0.5%) because the optical index $n_1$ of the DARC$_1$ is higher has $n_2$ of the DARC$_2$. 

![Fig.3. Losses of reflected flux of DARC$_1$ a function of wavelengths](image-url)

![Fig. 4. Losses of reflected flux of DARC$_2$ a function of wavelengths](image-url)
Fig. 5 Absorption losses as a function of wavelengths of DARC$_1$ and DARC$_2$

Fig. 6. Loss of absorption flux of Double layer DARC$_1$ and DARC$_2$

Fig. 6 shows the different absorption flux losses and photon flux density $F(\lambda)$ of the solar spectrum of AM1.5 G in DARC$_1$ and DARC$_2$. We note that the absorption losses in the UV range of the spectrum is considerably important and dominates all the losses in the DARC. The influence of refractive indices $n_1$ and $n_2$ layers DARC$_1$ ($d_1 = 58$ nm and $d_2 = 43$ nm) and DARC$_2$ ($d_1 = 76$ nm and $d_2 = 48$ nm) is illustrated in Fig. 7 and Fig. 8 respectively. Reflectivity of the materials used principally will depend on their optical indices when these indices are large, highly reflective layers in the visible and highly absorbent, which increases the losses by reflection and absorption, thus optimizing index $n_1$ and $n_2$ is necessary. For DARC$_1$ (Fig. 7) are the minimum reflectivity for small indices $n_1$ and $n_2$ large but this creates a strong absorption (see Fig. 5).

Fig. 7. Contour plot showing the total reflectance for different combinations of refractive index $n_1$ and $n_2$ for DARC$_1$ (SiN-SiN)

Fig. 8. Contour plot showing the total reflectance for different combinations of refractive index $n_1$ and $n_2$ for DARC$_2$ (SiN-SiO$_2$)

The DARC$_2$ (Fig. 8) seems a good compromise between the minimization of optical losses by reflection and absorption. It will therefore be necessary in the future to make a solar cell with such DARC and confirm the possible improvement of short-circuit. However, the thicknesses needed to achieve the DARC are relatively large for this; it will also ensure that these thicknesses are not a problem when making contacts through it.

5. Electrical results

The reflectivity spectra of DARC$_1$ and DARC$_2$ we had were incorporated into the database PC1D simulator, these simulations have enabled us to compare the electrical characteristics of cells, for both solar cell structures were based on the standard model of the simulator PC1D develop a material with low cost silicon solar cell. The parameters used are grouped in Table 2.
Finally, the application of a double layer antireflection the practically possible to win again of 1.8% and 3.3% of the short circuit a cell with a non-encapsulated and DARC1 and DARC2 respectively compared to a reference cell (SARC).

6. Conclusion

To increase the performances of the solar cells, we made a study of simulation two types different from the double antireflection layers, DARC1 (with the silicon nitride for the two layers) and the DARC2 (the silicon nitride and silicon oxide). The results of simulation went up that the choice of the layer of SiN is very important because of its great absorption for optical index high, for this reason, none combination of the DARC1 gives an important improvement of the current of short-circuit. However, the combination of two layers of SiN and SiO2 (DARC2) showed a clear improvement of current of short-circuit (3.3%) for non-encapsulated solar cells. Thus an application of a double antireflection layer of type DARC2 must be carried out and check these theoretically found results, and study its contribution to the improvement of current of short-circuit for encapsulated solar cells.

Reference


